

Nonequilibrium density operator approach to domain wall resistivity

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Abstract. We derive the static resistivity due to the Bloch domain wall using the nonequilibrium density operator technique by Zubarev in the ballistic limit of electronic transport.

An electronic transport in magnets with an inhomogeneous magnetic order is an active research topic due to promising applications in spintronics. A presence of a domain wall (DW) in a ferromagnet enables to control a DW motion by a spin polarized current of conducting electrons flowing through the domain wall [1]. A feedback effect is a change of transport properties that has been observed in a number of experiments. The excess resistivity due to DW (DWR) has been a subject of a number of studies. The most relevant theoretical treatments of DWR are based on the following concepts. (i) The mixing of spin states due to the magnetization twist in the DW [2]. The phenomenological spin dependent *impurity* scattering mixes the two-spin channels. The extra resistivity arises since the channels exhibit unequal conductivities in a ferromagnet in the absence of the wall. (ii) A redistribution of the charge carriers between spin-majority and spin minority channels due to the *domain wall* scattering [4, 5]. The works perform a diagrammatic evaluation of the Kubo's formula over the DW scattering potential. The *impurity* scattering is introduced in the unperturbed Green's functions through two phenomenological parameters, the momentum scattering times for spin-up and spin-down channels. (iii) A destruction of the weak localization corrections to conductivity by the domain wall [3]. It was shown that a DW contributes to the decoherence of electrons, leading to a decrease of the resistance. (iv) Spin accumulation around the DW which leads to an additional potential drop [6, 7, 8].

In the present paper we propose a microscopic calculation of the Bloch DW resistivity using the nonequilibrium density operator technique in the ballistic regime of electronic transport, when the electron mean free path is longer than the system size. The approach takes into account a domain-wall scattering [type-(ii) theory], but it is valid in the clean limit (the electronic relaxation time $\tau \rightarrow \infty$), where the resistivity is dominated by a spin structure. The case has been previously addressed by using the Mori formula [9].

We use the following model Hamiltonian to describe the system of conduction electrons

$$\hat{\mathcal{H}} = - \sum_{\langle i,j \rangle, \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} - \mu \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} - J_{sd} \sum_i \mathbf{S}_i \cdot \mathbf{s}_i, \quad (1)$$

where t_{ij} is a hopping integral between the nearest neighbour sites, μ is the chemical potential, $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) is an electron creation (annihilation) operator at the site i with spin $\sigma = \uparrow, \downarrow$. The

conduction electrons interact with the inhomogeneous magnetic texture via the sd exchange interaction with the coupling strength $J_{sd} > 0$, $\mathbf{S}_i = S(\cos \varphi_i \sin \theta_i, \sin \varphi_i \sin \theta_i, \cos \theta_i)$ denotes the localized spin of the texture parametrized by the polar angles θ and ϕ . The local spin of conduction electrons $\mathbf{s}_i = (1/2) \sum_{\sigma\sigma'} c_{i\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} c_{i\sigma'}$ is treated as a quantum operator, where $\boldsymbol{\sigma}$ stands for Pauli matrices.

Since the length scale of the DW is very large compared with the length scale of the electron (~ 0.1 nm at the Fermi level), the back reflection of free carriers by the DW can be ignored [10] and one can use the "adiabatic frame" approximation to study electron transport in such a slow varying in space magnetic background [9, 11].

The first step of analysis is to perform a local SU(2) unitary transformation $c_{i\sigma} = \sum_{\sigma'} (\hat{U}_i)_{\sigma\sigma'} b_{i\sigma}$, which removes the inhomogeneity of \mathbf{S}

$$\hat{U}_i^{-1}(\mathbf{S}_i \cdot \boldsymbol{\sigma}) \hat{U}_i = S\sigma_z. \quad (2)$$

The transformation matrix is given by $\hat{U}_i = \mathbf{m}_i \cdot \boldsymbol{\sigma}$ with the unit vector

$$\mathbf{m}_i = (\cos \varphi_i \sin \frac{\theta_i}{2}, \sin \varphi_i \sin \frac{\theta_i}{2}, \cos \frac{\theta_i}{2}). \quad (3)$$

Applying the local unitary rotation to the kinetic part of the Hamiltonian (1) and using the identity

$$\hat{U}_i^{-1} \hat{U}_{i+a_\nu} = 1 + i a_\nu (\mathbf{A}_\nu(\mathbf{r}_i) \cdot \boldsymbol{\sigma}) + o(A^2), \quad (4)$$

where a_ν is the lattice spacing along the ν axis, and

$$\mathbf{A}_\nu(\mathbf{r}_i) = [\mathbf{m}(\mathbf{r}_i) \times \partial_\nu \mathbf{m}(\mathbf{r}_i)] \quad (5)$$

is the non-Abelian gauge field created by the non-uniform magnetic texture ($\nu = x, y, z$), we obtain the Hamiltonian in the rotated frame as $\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{int}$.

After the Fourier transformations

$$b_{i\sigma} = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_i} b_{\mathbf{k}\sigma}, \quad \mathbf{A}_\nu(\mathbf{q}) = \frac{1}{V} \sum_{\mathbf{r}_i} e^{i\mathbf{q}\mathbf{r}_i} \mathbf{A}_\nu(\mathbf{r}_i), \quad (6)$$

the first part is given by

$$\hat{\mathcal{H}}_0 = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}\sigma} b_{\mathbf{k}\sigma}^\dagger b_{\mathbf{k}\sigma} \quad (7)$$

with the quasiparticle energies

$$\varepsilon_{\mathbf{k}\sigma} = -2 \sum_{\nu=1}^3 t_\nu \cos(k_\nu a_\nu) - \sigma M - \mu, \quad (8)$$

where $M = J_{sd}S/2$ is half the exchange splitting, and t_ν is the hopping integral along the ν axis in the real space.

The interaction part has the form

$$\hat{\mathcal{H}}_{int} = \hbar \sum_{\nu, \alpha} \sum_{\sigma\sigma'} \sum_{\mathbf{k}, \mathbf{k}'} A_\nu^\alpha(\mathbf{k}' - \mathbf{k}) \sigma_{\sigma\sigma'}^\alpha e^{\frac{i}{2}(k'_\nu - k_\nu)a_\nu} v_\nu \left(\frac{\mathbf{k}' + \mathbf{k}}{2} \right) b_{\mathbf{k}\sigma}^\dagger b_{\mathbf{k}'\sigma'}, \quad (9)$$

where the group velocity is

$$v_\nu(\mathbf{k}) = \frac{1}{\hbar} \frac{\partial \varepsilon_{\mathbf{k}\sigma}}{\partial k_\nu} = \frac{2}{\hbar} t_\nu a_\nu \sin(k_\nu a_\nu). \quad (10)$$

After the rotation the Hamiltonian (1) is transformed to that of electrons uniformly polarized and interacting with the SU(2) gauge field \mathbf{A} localized around the inhomogeneity [9]. The non-adiabaticity causes a scattering between the spin-up and spin-down channels and plays a role of spin-dependent scattering potential.

The current operator is

$$\mathbf{J} = e \sum_{\mathbf{k}\sigma} \mathbf{v}(\mathbf{k}) b_{\mathbf{k}\sigma}^\dagger b_{\mathbf{k}\sigma}, \quad (11)$$

where $e < 0$ is the electron charge. Its time derivative is

$$\dot{\mathbf{J}} = \frac{i}{\hbar} [\hat{\mathcal{H}}, \mathbf{J}] = ie \sum_{\alpha, \nu} \sum_{\mathbf{k}\sigma} \sum_{\mathbf{k}'\sigma'} A_\nu^\alpha(\mathbf{k}' - \mathbf{k}) \sigma_{\sigma\sigma'}^\alpha e^{\frac{i}{2}(k'_\nu - k_\nu) a_\nu} v_\nu \left(\frac{\mathbf{k}' + \mathbf{k}}{2} \right) (\mathbf{v}(\mathbf{k}') - \mathbf{v}(\mathbf{k})) b_{\mathbf{k}\sigma}^\dagger b_{\mathbf{k}'\sigma'}. \quad (12)$$

The dynamical resistivity per volume in isotropic materials obtained within the nonequilibrium density operator method [12] is given by

$$\rho(\omega) = \frac{3k_B T}{(\mathbf{J}, \mathbf{J})} \left[-i\omega + \frac{\langle \dot{\mathbf{J}}; \dot{\mathbf{J}} \rangle_{\omega+i\varepsilon}}{(\mathbf{J}, \mathbf{J}) + \langle \dot{\mathbf{J}}; \dot{\mathbf{J}} \rangle_{\omega+i\varepsilon}} \right], \quad (13)$$

where T is the temperature and k_B is the Boltzmann constant. In contrast to Kubo's formula for a linear response of isolated systems, Eq.(13) describes a response of open systems that in contact with a heat bath. What concerns external mechanical perturbations (for instance, electric or magnetic fields) the both approaches are equivalent. However, the method of the nonequilibrium density operator is naturally extended to thermal perturbations (f.e., local fluctuations of temperature or chemical potential) [12].

Provided the *adiabatic condition*, $M/t_\nu \gg a_\nu/\lambda_0$, where λ_0 is a scale of magnetic inhomogeneity, that means a smoothness of a spin texture, the time derivative (12) becomes a small parameter of the theory. This makes (13) is more convenient to evaluate the resistivity in comparison with the linear response theory, where an interaction with the gauge field is treated by using the standard diagrammatic perturbation theory [3].

The resistivity includes the static correlation function of the current operators

$$(\mathbf{J}, \mathbf{J}) = \sum_{\alpha=x,y,z} \int_0^1 dx \text{Tr} \{ \mathbf{J}_\alpha \mathbf{J}_\alpha (i\hbar\beta x) \rho_0 \}, \quad (14)$$

where $\beta = 1/(k_B T)$, $\rho_0 = \exp(-\beta\hat{\mathcal{H}}) / \text{Tr} \exp(-\beta\hat{\mathcal{H}})$ is the equilibrium density matrix and $\mathbf{J}_\alpha(i\hbar\beta x) = e^{-\beta x \hat{\mathcal{H}}} \mathbf{J}_\alpha e^{\beta x \hat{\mathcal{H}}}$.

The symbol $\langle \dots \rangle$ represents the Laplace transform of the time correlation function

$$\langle A; B \rangle_{\omega+i\varepsilon} = \int_0^\infty dt e^{i(\omega+i\varepsilon)t} (A(t), B), \quad (15)$$

where A, B mean either \mathbf{J} or $\dot{\mathbf{J}}$ operators.

In the following we consider the static resistivity at $\omega = 0$ and focus on spin textures varying only in one spacial direction, say along the z axis, and uniformly magnetized within the perpendicular xy plane. Then, $\mathbf{A}_\nu(\mathbf{q}) \rightarrow A_z(q_z)$. Likewise we assume that electrons move only along the selected direction with the energy $\varepsilon_{k_z\sigma} = -2t_z \cos(k_z a_z) - \sigma M - \mu$, i.e. the hopping terms t_x, t_y are neglected and the factor 3 in Eq.(13) should be omitted.

Plugging the expression in Eqs.(17,15) we get

$$\begin{aligned} \langle \dot{J}_z; \dot{J}_z \rangle_{i\varepsilon} &= \pi \hbar e^2 \sum_{\alpha_1 \alpha_2} \sum_{k_1 \sigma_1} \sum_{k'_1 \sigma'_1} A_z^{\alpha_1}(k'_1 - k_1) A_z^{\alpha_2}(k_1 - k'_1) \sigma_{\sigma_1 \sigma'_1}^{\alpha_1} \sigma_{\sigma'_1 \sigma_1}^{\alpha_2} \\ &\times v_z^2 \left(\frac{k'_1 + k_1}{2} \right) \left(v_z(k'_1) - v_z(k_1) \right)^2 f_{k_1 \sigma_1} (1 - f_{k'_1 \sigma'_1}) \delta(\varepsilon_{k_1 \sigma_1} - \varepsilon_{k'_1 \sigma'_1}), \end{aligned} \quad (16)$$

and after some calculations the expression is simplified to be

$$\langle \dot{J}_z; \dot{J}_z \rangle_{i\varepsilon} = 2\pi \hbar e^2 \sum_{kk'} A_z^{(-)}(k' - k) A_z^{(+)}(k - k') v_z^2 \left(\frac{k' + k}{2} \right) \left(v_z(k') - v_z(k) \right)^2 f_{k\uparrow} (1 - f_{k'\uparrow}) \delta(\varepsilon_{k\uparrow} - \varepsilon_{k'\downarrow}), \quad (17)$$

where $A_z^{(\pm)} = A_z^x \pm i A_z^y$. As is obvious, the spin flip scattering of conduction electrons is provided by the transverse components of the gauge field.

The static correlation function is obtained as

$$(J_z, J_z) = e^2 \sum_{k\sigma} v_z^2(k) f_{k\sigma} (1 - f_{k\sigma}), \quad (18)$$

where $f_{k\sigma} = (\exp \beta \varepsilon_{k\sigma} + 1)^{-1}$ is the Fermi distribution function. By the same manner we get the trivial result $\langle \dot{J}_z; J_z \rangle_{i\varepsilon} = 0$.

Replacing in Eqs.(17,18) the sums over k by the appropriate integrals $\sum_k \rightarrow a_z/(2\pi) \int_{BZ} dk$ and carrying out straightforward calculations we get the eventual result for the dc resistivity per volume

$$\rho = \frac{\hbar k_B T M^2 \mathcal{K}_1}{2e^2 a_z^2 t_z^3 \mathcal{K}_2^2}. \quad (19)$$

Here we introduce the dimensionless quantities determined as

$$\mathcal{K}_1 = \frac{a_z}{2\pi} \sum_{\sigma} \int_{k_{\min}}^{\pi/a_z} dk \frac{\mathcal{A}(k - \sigma k_0) \cos^2(\{ka_z + \sigma k_0 a_z\}/2)}{[1 - \{M/t_z + \cos(ka_z)\}^2]^{1/2}} f_{k\uparrow} (1 - f_{k\uparrow}), \quad (20)$$

$$\mathcal{K}_2 = \frac{a_z}{2\pi} \sum_{\sigma} \int_{-\pi/a_z}^{\pi/a_z} dk \sin^2(ka_z) f_{k\sigma} (1 - f_{k\sigma}), \quad (21)$$

where $k_0 a_z = \cos^{-1}[M/t_z + \cos(ka_z)]$, $k_{\min} a_z = \cos^{-1}[1 - M/t_z]$, and

$$\mathcal{A}(q) = a_z^2 \left[A_z^{(+)}(q) A_z^{(-)}(-q) + A_z^{(+)}(-q) A_z^{(-)}(q) \right]. \quad (22)$$

The explicit form of $\mathcal{A}(q)$ depends on a spin configuration. In the case of the Bloch domain wall, $\varphi(z) = 2 \tan^{-1} e^{z/\lambda}$ and $\theta = \pi/2$, where λ is the thickness of the DW, it is given by

$$\mathcal{A}(q) = 2 (\pi q \lambda)^2 \frac{\cosh(\pi q \lambda)}{\sinh^2(\pi q \lambda)}. \quad (23)$$

The last result is derived by using the vector gauge field created by the Bloch DW

$$\mathbf{A}_z(z) = \frac{1}{2\lambda} \left(\frac{\sinh(z/\lambda)}{\cosh^2(z/\lambda)}, -\frac{1}{\cosh^2(z/\lambda)}, \frac{1}{\cosh(z/\lambda)} \right). \quad (24)$$

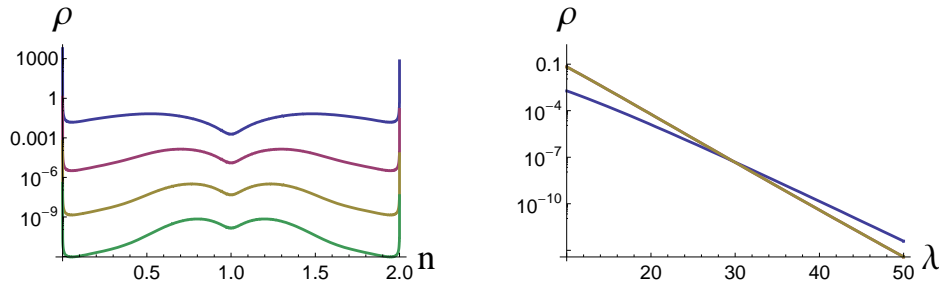


Figure 1. The static DW resistivity (in arb. units) at different domain wall thicknesses (λ varies from 10 till 40 with the step 10) as a function of the electronic concentration n (left panel). Dependence of ρ on the DW thickness for the concentrations $n = 0.5$ (or 1.5) and $n = 1$ (right panel). The parameters are chosen as $M/t_z = 0.2$, $k_B T/t_z = 0.1$ at $t_z = 1.0$.

The answer for the resistivity becomes transparent at zero temperature

$$\rho = \frac{\hbar \pi M^2}{e^2 a_z^2 t_z^2} \frac{\sum_{\sigma} \mathcal{A}(k_{F\uparrow} - \sigma k_{F\downarrow}) \cos^2([k_{F\uparrow} + \sigma k_{F\downarrow}]a_z/2)}{|\sin(k_{F\downarrow}a_z)| |\sin(k_{F\uparrow}a_z)| (\sum_{\sigma} |\sin(k_{F\sigma}a_z)|)^2}, \quad (25)$$

where $k_{F\sigma}$ is the Fermi momentum of the polarized electrons, i.e. the DW gauge field supports the spin-flip scattering of electrons at the Fermi level. We pay attention that spin flip processes *without momentum transfer* are responsible for an emergence of the spin-transfer torque from spins of itinerant electrons to local moments [11] whereas spin flip processes *with momentum transfer* results in the resistivity due to the DW.

The finite temperature resistivity is plotted in Fig.1 as a function of the electronic concentration per site n and the DW thickness λ . To obtain the dependencies we calculate the chemical potential from the condition $\sum_{k\sigma} f_{k\sigma} = n$, where $0 \leq n \leq 2$.

As a summary, by using the nonequilibrium density operator technique we have calculated the static domain-wall resistivity of a Bloch wall situated in a wire of quasi-one-dimensional geometry when the current flows perpendicularly to the wall plane.

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